

IN THE ABSTRACT:

Please replace the existing Abstract with the following Abstract.

A method and apparatus determine spatially similar portions of substances by analyzing three-dimensional structures of the substances including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set and automatically determining a distance between the elements of the first point set and the elements of the second point set that have an optimal correspondence. The method includes dividing the first point set and second point set into first subsets and second subsets; generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence; determining the optimum correspondence between the elements belonging to each pair of subsets; and calculating a root mean square distance between all of the elements corresponding in the optimum correspondence.